



# A new computational framework for atmospheric and surface remote sensing

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*supporting cast*

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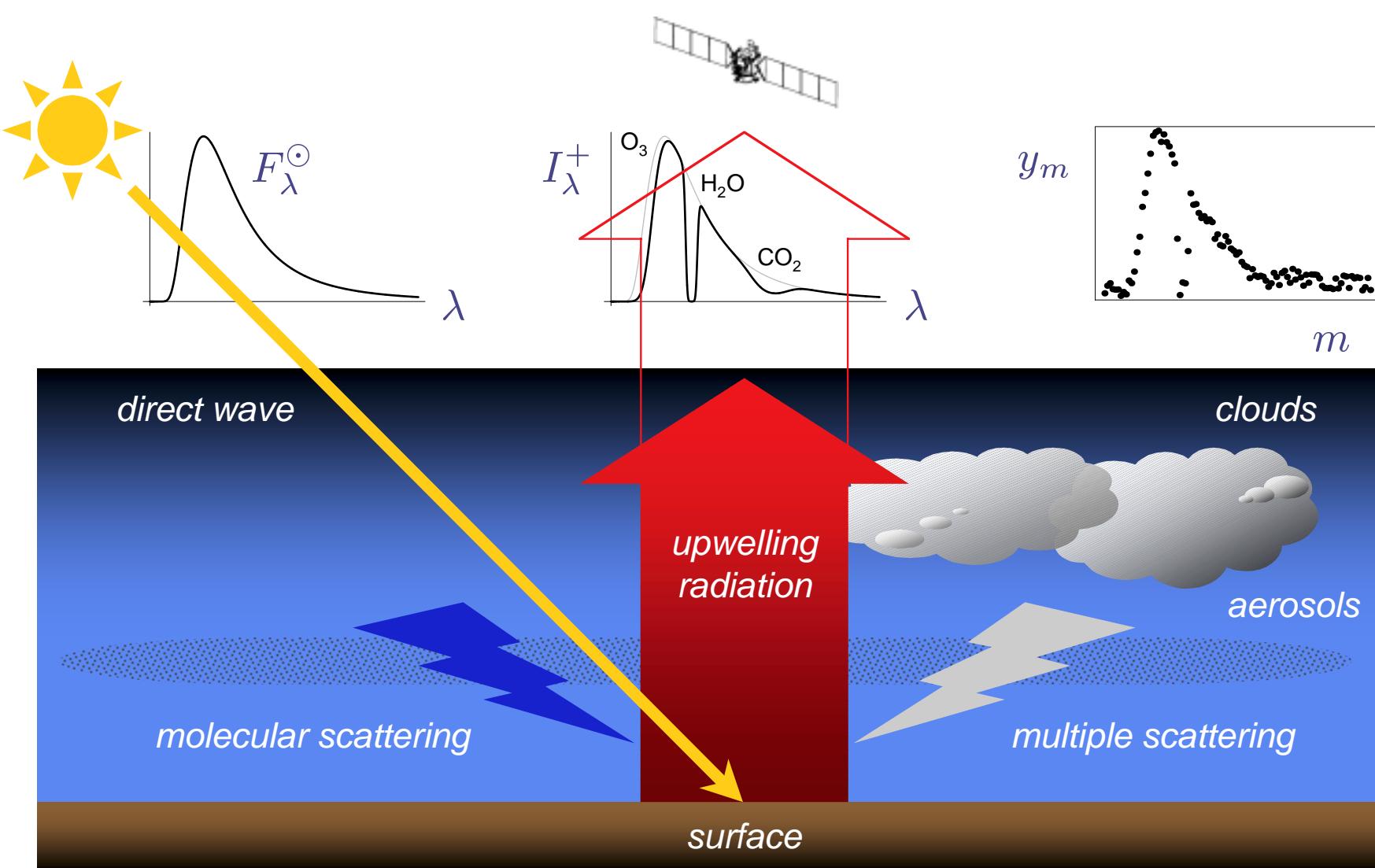
# Problem statement



*Simultaneous retrieval of  
atmospheric **and** surface composition  
from remotely-sensed hyper-spectral data*

*to help answer  
outstanding Earth-Science challenge questions  
chiefly related to the solar radiation budget*

# Hyper-spectral remote sensing



# The retrieval problem



- The “standard” (static) measurement model:

$$\mathbf{y} = \mathbf{f}(\mathbf{x}) + \boldsymbol{\epsilon}$$

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*state vector*

$$\mathbf{x} = \{x_n, n = 1, 2, \dots, N\}$$

*measurement vector*

$$\mathbf{y} = \{y_m, m = 1, 2, \dots, M\}$$

*forward model*

$$\mathbf{f} : \mathbb{R}^N \mapsto \mathbb{R}^M$$

*random noise*

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$$\boldsymbol{\epsilon} = \{\epsilon_m, m = 1, 2, \dots, M\}$$

- The “inverse” problem:

*estimate unknowns  $\mathbf{x}$  from measurements  $\mathbf{y}$*

- the curse of dimensionality:  $N \sim \mathcal{O}(10^2)$

# Research objectives

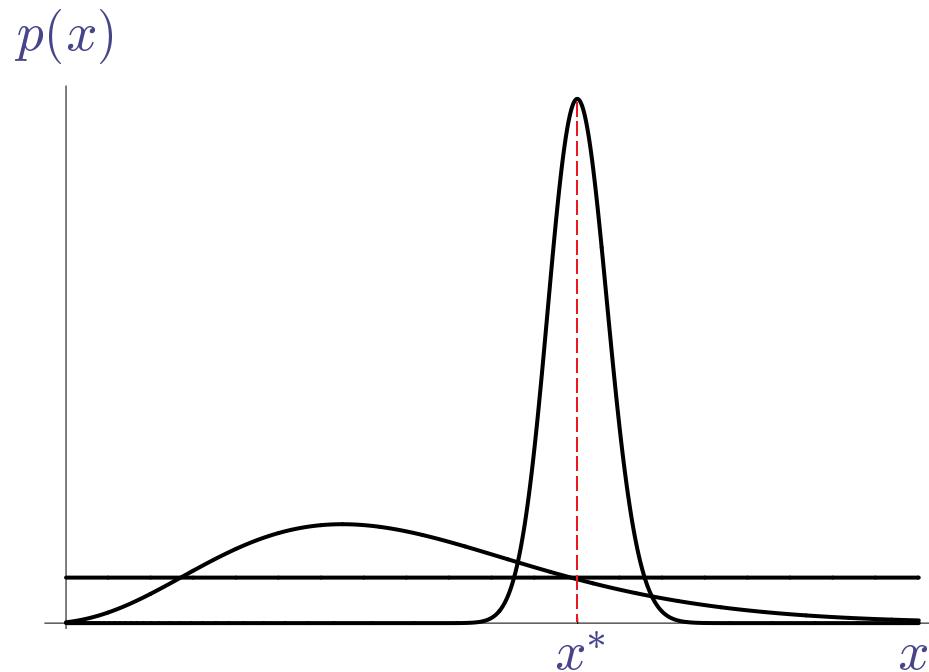


- Simultaneous retrieval of
$$\{T(z), P(z), N_i(z), \rho_\lambda(\hat{s}; \hat{s}'), \dots\}$$
  - bridge the gaps between
    - atmospheric and surface remote-sensing
    - physical modeling and data analysis
- Improved accuracy in forward models and retrievals
  - crucial for resolving instrument cross-validation issues
  - necessary for enhancing predictive power of GCMs
- Main practical questions:
  - do we (now) have enough computational power?
  - is an hyper-spectral data set sufficient for doing this?

# Bayesian inference



- State of knowledge as a probability distribution:



- Bayes' theorem:

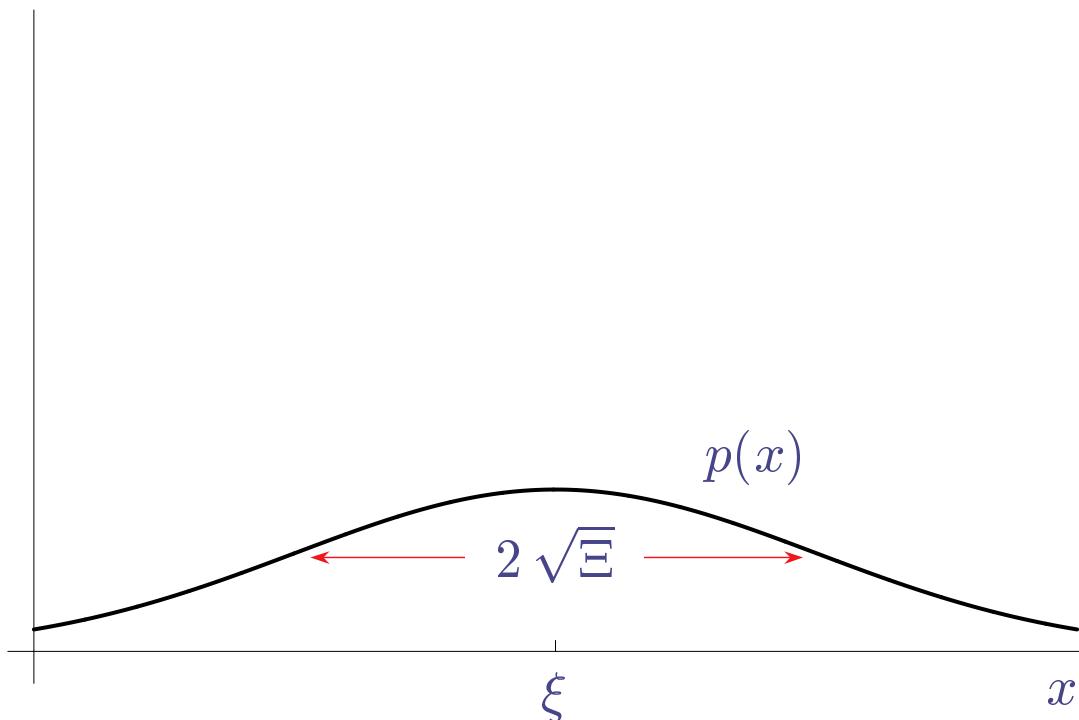
$$p(\text{model}|\text{data}) = \frac{p(\text{data}|\text{model}) p(\text{model})}{p(\text{data})}$$

# Bayesian inference



- State prior – initial best guess  $\xi$  and uncertainty  $\Xi$ :

$$p(\mathbf{x}) \propto \exp \left[ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\xi})^T \boldsymbol{\Xi}^{-1} (\mathbf{x} - \boldsymbol{\xi}) \right]$$

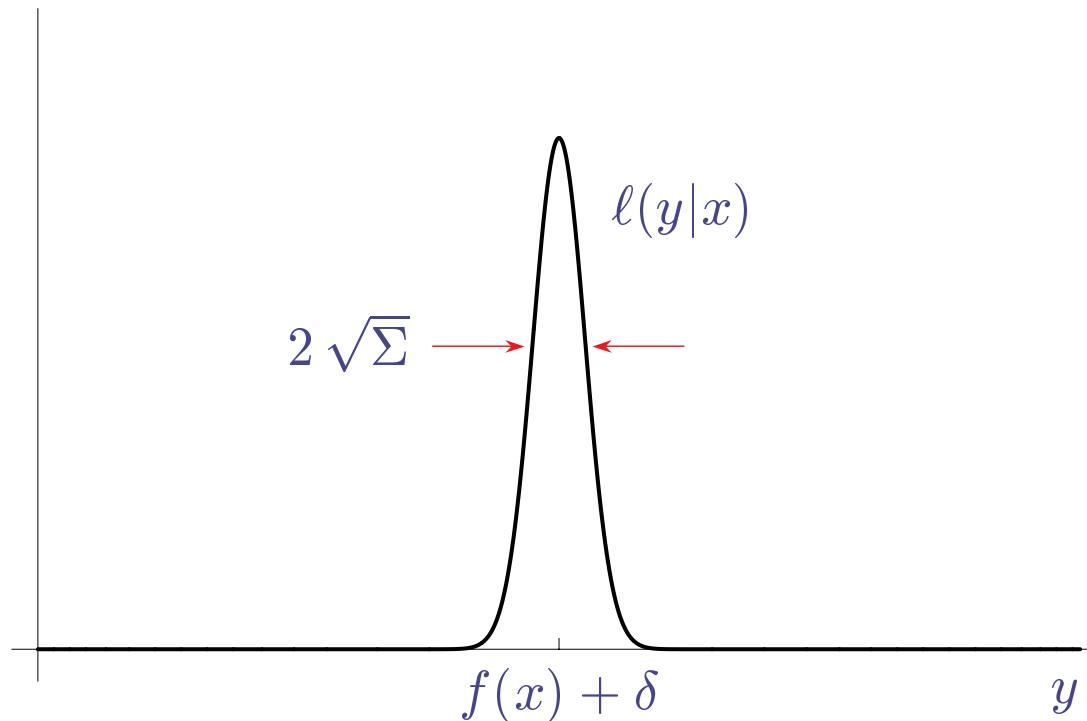


# Bayesian inference



- Measurement likelihood – Gaussian noise  $\epsilon \sim \mathcal{N}(\delta, \Sigma)$ :

$$\ell(\mathbf{y}|\mathbf{x}) \propto \exp \left\{ -\frac{1}{2} [\mathbf{y} - \mathbf{f}(\mathbf{x}) - \boldsymbol{\delta}]^T \boldsymbol{\Sigma}^{-1} [\mathbf{y} - \mathbf{f}(\mathbf{x}) - \boldsymbol{\delta}] \right\}$$

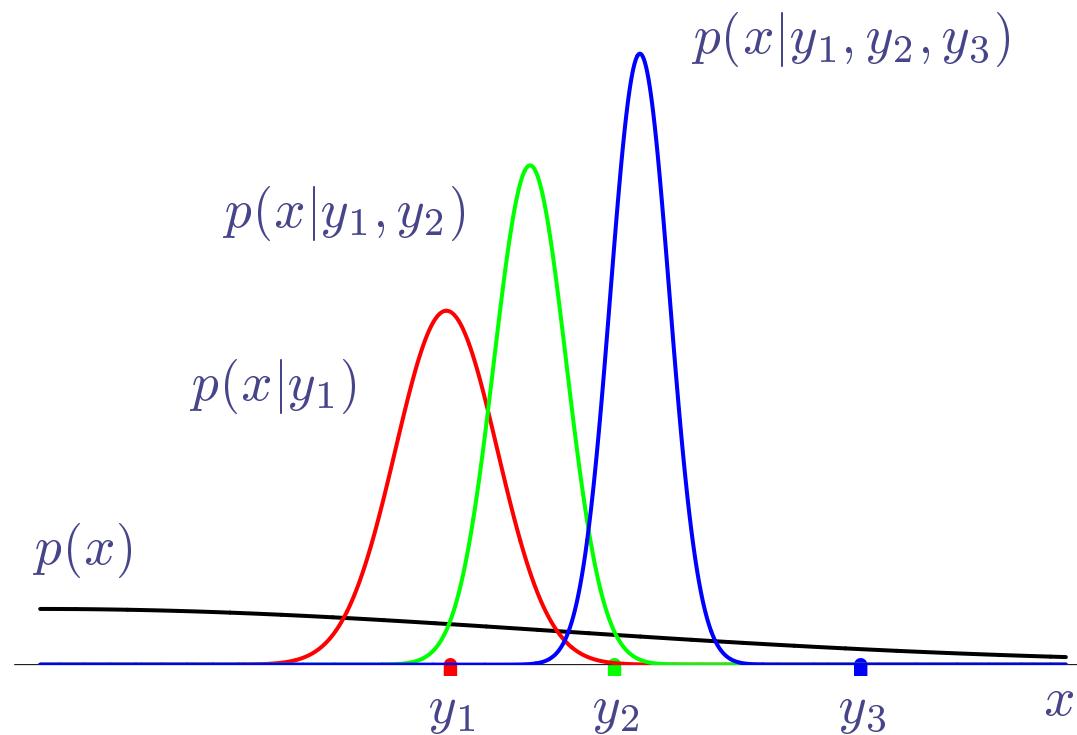


# Bayesian inference



- State posterior via Bayes' theorem:

$$p(\mathbf{x}|\mathbf{y}) = \frac{\ell(\mathbf{y}|\mathbf{x}) p(\mathbf{x})}{p(\mathbf{y})} = \frac{\ell(\mathbf{y}|\mathbf{x}) p(\mathbf{x})}{\int \ell(\mathbf{y}|\mathbf{x}) p(\mathbf{x}) d\mathbf{x}}$$



# Optimal estimation



- “Cost” function:

$$\begin{aligned} J(\mathbf{x}) &\equiv -\ln \ell(\mathbf{y}|\mathbf{x}) - \ln p(\mathbf{x}) \\ &= \frac{1}{2} [\mathbf{y} - \mathbf{f}(\mathbf{x}) - \boldsymbol{\delta}]^T \boldsymbol{\Sigma}^{-1} [\mathbf{y} - \mathbf{f}(\mathbf{x}) - \boldsymbol{\delta}] \\ &\quad + \frac{1}{2} (\mathbf{x} - \boldsymbol{\xi})^T \boldsymbol{\Xi}^{-1} (\mathbf{x} - \boldsymbol{\xi}) + C \end{aligned}$$

- Maximum *a posteriori* estimate  $\mathbf{x}^*$ :

$$J(\mathbf{x}^*) \leq J(\mathbf{x}) \quad \forall \mathbf{x} \neq \mathbf{x}^*$$

- Multi-dimensional “error bar”  $\mathbf{S}^*$ :

$$\ln p(\mathbf{x}|\mathbf{y}) = \ln p(\mathbf{x}^*|\mathbf{y}) - \frac{1}{2} (\mathbf{x} - \mathbf{x}^*)^T \mathbf{S}^{*-1} (\mathbf{x} - \mathbf{x}^*) + \dots$$

# Practical optimization



- simulated annealing – only requires  $f(\mathbf{x})$
- Gauss–Newton (with Levenberg–Marquardt)
  - start with  $\mathbf{x}_0 = \boldsymbol{\xi}$

$$\begin{aligned}\mathbf{x}_{k+1} &= \mathbf{x}_k - (\mathbf{K}_k^T \Sigma^{-1} \mathbf{K}_k + \boldsymbol{\Xi}^{-1})^{-1} \\ &\quad \cdot \left[ \boldsymbol{\Xi}^{-1} (\mathbf{x}_k - \boldsymbol{\xi}) - \mathbf{K}_k^T \Sigma^{-1} (\mathbf{y} - \mathbf{f}_k - \boldsymbol{\delta}) \right] \rightarrow \mathbf{x}^* \\ \mathbf{S}_k &= (\mathbf{K}_k^T \Sigma^{-1} \mathbf{K}_k + \boldsymbol{\Xi}^{-1})^{-1} \rightarrow \mathbf{S}^*\end{aligned}$$

- additionally requires the Jacobian matrix

$$\mathbf{K}(\mathbf{x}) \equiv \nabla \mathbf{f}(\mathbf{x}) = \left\{ \frac{\partial f_m(\mathbf{x})}{\partial x_n} \right\}$$

# Remote-sensing data analysis



## • Generalization

- multiple measurements  $\mathbf{y}_a$  (length  $M_a$ )
  - hyper-spectral image pixels
  - alternative multi-spectral radiometer data
  - *in situ* (aircraft, sonde, etc.) measurements
  - active (radar, lidar, etc.) measurements . . .
  - full set of data  $\mathbb{Y} = \{\mathbf{y}_a\}$
- multiple unknown states  $\mathbf{x}_b$  (length  $N_b$ )
  - thermodynamic properties
  - vertical trace-gas concentration profiles
  - cloud and aerosol micro-physical properties
  - surface spectral and angular reflectance . . .
  - full set of unknowns  $\mathbb{X} = \{\mathbf{x}_b\}$

# Remote-sensing data analysis



- Bayes' theorem (with independent measurements):

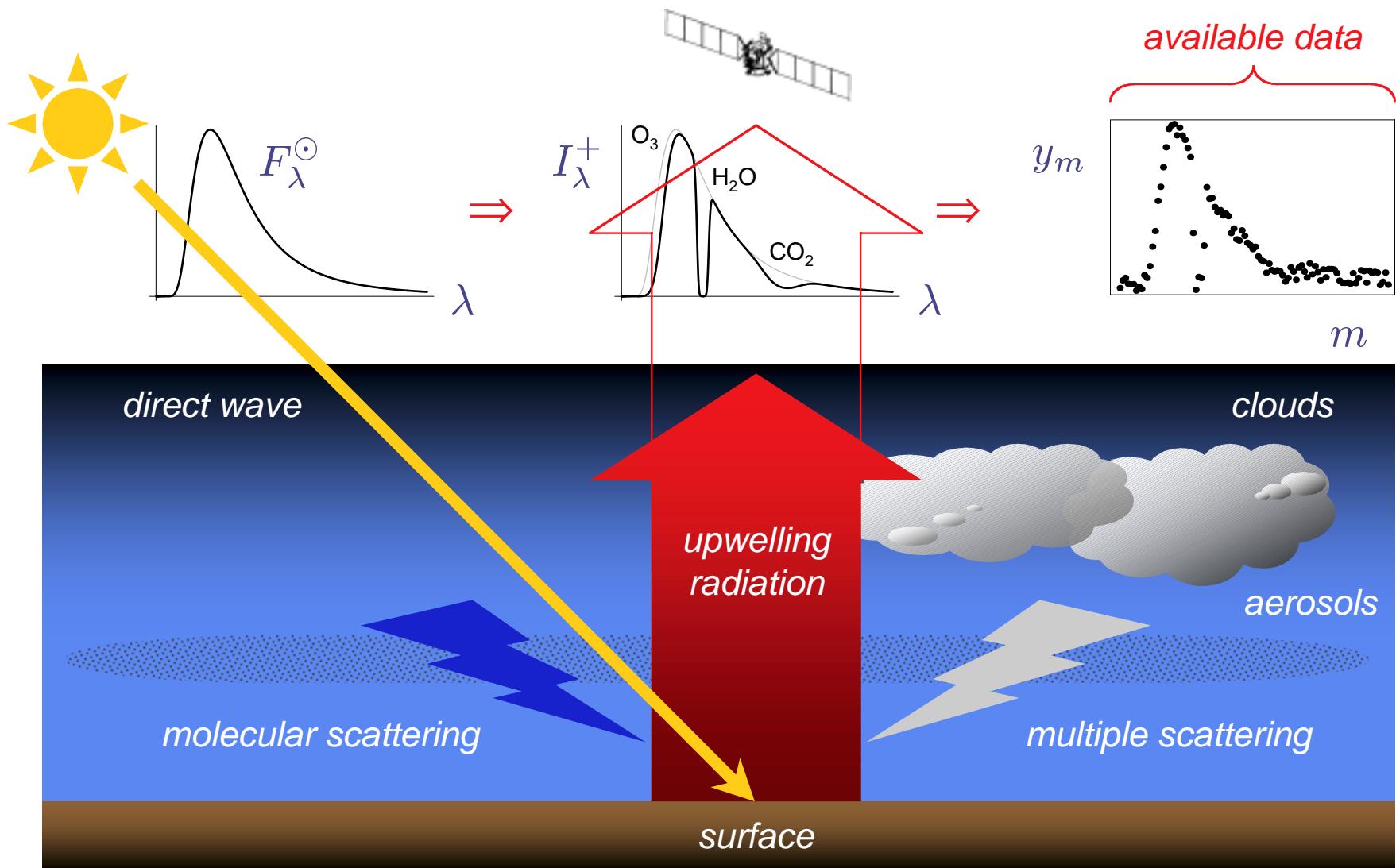
$$p(\mathbb{X}|\mathbb{Y}) = \frac{\ell(\mathbb{Y}|\mathbb{X}) p(\mathbb{X})}{p(\mathbb{Y})} = \frac{1}{p(\mathbb{Y})} \prod_a \ell(\mathbf{y}_a|\mathbb{X}) \prod_b p(\mathbf{x}_b)$$

- Full cost function (with Gaussian PDFs):

$$\begin{aligned} J(\mathbb{X}) &= -\ln \ell(\mathbb{Y}|\mathbb{X}) - \ln p(\mathbb{X}) \\ &= \frac{1}{2} \sum_a [\mathbf{y}_a - \mathbf{f}_a(\mathbb{X}) - \boldsymbol{\delta}_a]^T \boldsymbol{\Sigma}_a^{-1} [\mathbf{y}_a - \mathbf{f}_a(\mathbb{X}) - \boldsymbol{\delta}_a] \\ &\quad + \frac{1}{2} \sum_b (\mathbf{x}_b - \boldsymbol{\xi}_b)^T \boldsymbol{\Xi}_b^{-1} (\mathbf{x}_b - \boldsymbol{\xi}_b) + C' \end{aligned}$$

- minimize to find  $\mathbb{X}^*$

# Forward models



# Sensor model



- Hyper-spectral instrument:  $M$  bands over  $(\lambda_{\min}, \lambda_{\max})$

$$y_m = \left. \beta_m \int_{\Delta\lambda} \psi(\lambda_m - \lambda) \int_{2\pi} \chi(\hat{\mathbf{n}} \cdot \hat{\mathbf{s}}) I_\lambda^+(\mathbf{r}, \hat{\mathbf{s}}; \mathbb{X}) d\Omega d\lambda \right\} f_m(\mathbb{X}) + (\delta_m + \eta_m) \quad \right\} \epsilon_m$$

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<i>center, gain, offset, noise</i>	$\lambda_m, \beta_m, \delta_m, \eta_m$
<i>spectral resolution</i>	$\Delta\lambda$
<i>slit function</i>	$\psi(\lambda)$
<i>point-spread function</i>	$\chi(\cos \Theta)$
<i>upwelling spectral radiance</i>	$I_\lambda^+(\mathbf{r}, \hat{\mathbf{s}}; \mathbb{X})$

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- Unknown / changing instrument parameters:  $\mathbf{x}_{\text{ins}} \in \mathbb{X}$

# Molecular atmosphere



- State vectors:  $\mathbf{x}_b = \{b_l \equiv b(z_l)\}, b = T, P, N_i$
- Layer optical depths: Voigt profile via FFT

$$\tau_l(\nu) = \int_{-\infty}^{\infty} dt e^{i2\pi\nu t} \int_{z_{l-1}}^{z_l} dz \sum_i N_i(z) \sum_j S_{ij}(z) \cdot \exp \left\{ -i2\pi\nu_{ij}(z)t - 2\pi\hat{\gamma}_{ij}(z)|t| - [\pi\tilde{\gamma}_{ij}(z)t]^2 \right\}$$

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<i>resonance line center</i>	$\nu_{ij}(P)$
<i>resonance line strength</i>	$S_{ij}(T)$
<i>impact-induced line width</i>	$\hat{\gamma}_{ij}(T, P, N_i)$
<i>motion-induced line width</i>	$\tilde{\gamma}_{ij}(T)$

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# Molecular atmosphere



- Line parameters: obtain from a spectral database\*

$$\nu_{ij}(P) = \nu_{ij}^* + \delta_{ij}^* P$$

$$S_{ij}(T) = S_{ij}^* \left( \frac{T^*}{T} \right)^{m_i^*} \exp \left[ -\frac{h_P c}{k_B} E_{ij}^* \left( \frac{1}{T} - \frac{1}{T^*} \right) \right]$$

$$\hat{\gamma}_{ij}(T, P, N_i) = \left( \frac{T^*}{T} \right)^{n_i^*} [\hat{\gamma}_{ij}^* P + (\hat{\gamma}'_{ij}^* - \hat{\gamma}_{ij}^*) N_i k_B T]$$

$$\tilde{\gamma}_{ij}(T) = \frac{\nu_{ij}^*}{c} \sqrt{\frac{2 N_A k_B T}{M_i}}$$

- Vertical profiles: fit with cubic splines
  - low-dimensional representation, analytic  $z$  integration

# Radiative transfer model



- Radiance  $I_\nu(\tau, \mu, \phi)$  in a plane-parallel atmosphere:

$$\mu \frac{\partial I_\nu}{\partial \tau} = I_\nu(\tau, \mu, \phi)$$

$$- \varpi_\nu(\tau) \int_0^{2\pi} \int_{-1}^1 p(\mu, \phi; \mu', \phi') I_\nu(\tau, \mu', \phi') d\mu' d\phi'$$

- albedo  $\varpi_\nu(\tau)$  from quantum physics or spectroscopy
- phase function  $p(\hat{s}; \hat{s}')$  from Rayleigh scattering
- boundary conditions – TOA:  $\tau = 0$ ; surface:  $\tau = \bar{\tau}$

$$I_\nu^-(0, \mu, \phi) = F_\nu^\odot \delta(\mu - \mu^\odot) \delta(\phi - \phi^\odot)$$

$$I_\nu^+(\bar{\tau}, \mu, \phi) = \int_0^{2\pi} \int_{-1}^0 \rho_\nu(\mu, \phi; \mu', \phi') I_\nu^-(\bar{\tau}, \mu', \phi') \mu' d\mu' d\phi'$$



- Forward model
  - molecular parameters from HITRAN database
  - solar spectral flux  $F_\nu^\odot$  via Kurucz model
  - radiance  $I_\lambda^+(\mathbf{r}, \hat{\mathbf{s}}; \mathbb{X})$  via DISORT code
- Retrieval algorithm
  - priors  $\xi_b$  from 1976 US Standard Atmosphere
  - ground truth from DoE ARM SGP site
- Future work
  - vectorial DISORT for full Stokes vector  $\mathbf{I}_\lambda^+(\mathbf{r}, \hat{\mathbf{s}}; \mathbb{X})$
  - linearized DISORT for fast Jacobians  $\mathbf{K}_a(\mathbf{x}_b)$
  - Target datasets: *MODIS*, *Hyperion*, *AVIRIS*

# Conclusions



- Bayesian setting: *emphasize model over data*
  - domain knowledge and expertise enter naturally through priors and likelihoods
  - enables real-time processing of “streaming” data
  - enables assessment of parametric uncertainties
    - prevent data volume from growing unnecessarily
  - heterogeneous data analyzed in the context of a common physical model
    - seamless integration of data from multiple sensors (after registration!)
    - collaboration instead of competition / conflict between sensors

# Conclusions



- Forward models: *sensor plus atmosphere–surface*
  - unified sensor / measurement model
    - reduces instrument disagreements
    - enables “on-line learning” of sensor parameters
  - full radiative transfer model
    - known physics provides strong constraint – our “best asset” for data analysis
    - model can be shared by all radiation sensors
    - high-accuracy framework for incorporating particle (cloud, aerosol) and surface scattering codes
    - enables **joint inference** of atmospheric and surface parameters